STRUCTURE FILE UPDATES: 19 SEP 2005 HIGHEST RN 863478-08-4 DICTIONARY FILE UPDATES: 19 SEP 2005 HIGHEST RN 863478-08-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

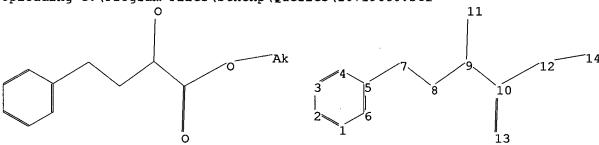
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Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>

Uploading C:\Program Files\Stnexp\Queries\10719660.str



chain nodes:
7 8 9 10 11 12 13 14

ring nodes:
1 2 3 4 5 6

chain bonds:
5-7 7-8 8-9 9-10 9-11 10-12 10-13 12-14

ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds:
9-11 10-12 10-13 12-14

exact bonds:
5-7 7-8 8-9 9-10

normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS

=> d L1 HAS NO ANSWERS L1 STR

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 16:16:38 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2151 TO ITERATE

93.0% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

50 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

PROJECTED ITERATIONS: 40238 TO 45802

PROJECTED ANSWERS: 653 TO 1541

L2 50 SEA SSS SAM L1

=> s 11 full FULL SEARCH INITIATED 16:16:43 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 43191 TO ITERATE

100.0% PROCESSED 43191 ITERATIONS. 1314 ANSWERS SEARCH TIME: 00.00.01

L3 1314 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
161.33
161.54

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FILE COVERS 1907 - 20 Sep 2005 VOL 143 ISS 13 FILE LAST UPDATED: 19 Sep 2005 (20050919/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13/p671 L3/P => s 13 and (process or make or made or synthes? or method) 819 L3 2147110 PROCESS 1436157 PROCESSES 3194259 PROCESS (PROCESS OR PROCESSES) 216040 MAKE 168027 MAKES 372909 MAKE (MAKE OR MAKES) 1166867 MADE 24 MADES 1166888 MADE (MADE OR MADES) 1476331 SYNTHES? 2940330 METHOD 1210143 METHODS 3810022 METHOD (METHOD OR METHODS) L5 446 L3 AND (PROCESS OR MAKE OR MADE OR SYNTHES? OR METHOD) => s 15 and (nitrile and acid) 55666 NITRILE 25916 NITRILES 70084 NITRILE (NITRILE OR NITRILES) 4035727 ACID 1492437 ACIDS 4518122 ACID

(ACID OR ACIDS)

L6 4 L5 AND (NITRILE AND ACID)

=> d ibib abs hitstr tot

L6 ANSYER 1 OF 4
ACCESSION NUMBER:
DOCUMENT NUMBER:
1111E: Process for producing erythro-3-amino-2hydroxybutyric acid derivatives
PUTUKAWA, Yoshiro: Yaegashi, Keisuker Hinoue, Kazumasa
DOCUMENT TYPE:
LANGUAGE: PATENT ACC. NUM. COUNT:
PATENT INFORMATION:

CAPLUS COPYRIGHT 2005 ACS on STN
2004:1002 CAPLUS
141:174475
Process for producing erythro-3-amino-2hydroxybutyric acid derivatives
Putukawa, Yoshiro: Yaegashi, Keisuker Hinoue, Kazumasa
Daiso Co., Ltd., Japan
Eur. Patent
Patent
Patent
Patent
Patent
INFORMATION:

COUNT:
3 PATENT NO. KIND DATE APPLICATION NO.

EP 1449824 Al 20040825 EP 2004-290653 20000622
R: CH, DE, FR, GB, LI
EP 1063232 A2 20001227 EP 2000-401792 20000622
EP 1063232 A3 20010307
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO
PRIORITY APPLN. INFO.:

EP 2000-401792 A 19990622
EP 2000-401792 A 19990622
EP 2000-401792 A 19990622 LV, FI, RO JP 1999-174967 EP 2000-401792 CASREACT 141:174475; MARPAT 141:174475 OTHER SOURCE(S):

A process for producing an erythro-3-amino-2-hydroxybutyric acid derivative involves reaction of a 2-amino aldehyde derivative I [R1 is alkyl, cycloalkyl, alkylthio, arythho or (un)substituted aryl; P1, P2 are (un)substituted aralkyl, alkylcxycarbonyl, arylcarbonyl or arylsulfonyl) with a metal cyanide in the presence of an acid chloride and/or an acid anhydride to give stereoselectively an erythro-3-amino-2-hydroxybutyronitrile derivative II [same R1, P1 and P2; R2 is alkylcarbonyl or (un)substituted arylcarbonyl group). The nitrile derivative II is treated with an acid in water or aqueous solvent to convert it into an erythro-3-amino-2-hydroxybutyric acid derivative III [same R1, R3 is H; O1, O2 are H, (un)substituted aralkyl or arylsulfonyl) or with an acid in an alc. solvent R3OH to convert it into an ester III [same R1, Q1 and Q2; R3 is alkyl, cycloalkyl or (un)substituted aralkyl under two-phase catalysis. Thus, the process was applied to the synthesis of Me (25, 35)-3-(dibenzylamino)-2-hydroxy-4-phenylbutycate (erythro:threo = 87:13, 73% yield) starting from N,N-dibenzyl-L-phenylalaninal.

L6 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 1993:560824 CAPLUS DOCUMENT NUMBER: 119:160824

TITLE:

INVENTOR(S):

119:160824

**Process for the preparation of a-hydroxy-\$\text{\$\text{\$P\$}\$ anids } \$\$\$ Baenziger, Markus; Warm, Aleksander; McGarrity, John Lonza A.-G., Switz.

**Euc. Pat. Appl., 10 pp.

COURM: EXEKUW PATENT ASSIGNEE(S): SOURCE:

Patent German

DOCUMENT TYPE: P:
LANGUAGE: GC
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

	PATENT NO.			APPLICATION NO.	DATE
	EP 543343	A2	19930526	EP 1992-119634	19921117
	EP 543343	A3	19930721		
	R: AT, BE, CH,	DE, FR,	GB, IT, LI,	NL, SE	
	JP 06184069	A2	19940705	JP 1992-303629	19921113
	CA 2083108	AA	19930520	CA 1992-2083108	19921117
PRIC	RITY APPLN. INFO.:			CH 1991-3373 A	19911119
OTHE	R SOURCE(S):	CASREAC	T 119:160824	; MARPAT 119:160824	
AB	R1CH (NR3R4) CH (OH) CO	2R2 [R1	 (substitut 	ed) alkvl; R2 = H, alk	rvl: R3. R4 =
				l protecting group), w	
				R3.R4, except that bo	
				give R1CH(NR5R6)COCN,	
)COCO2R7 (R7 = alkv1).	
	elective reduction of the keto group, and 4) optional deprotection/ester				
give 98% acid chloride, which was heated with Me3SICN and ZnI2					
	in 7HF to give 87% mitrile. This in Et20/MeOH/HCl was stirred				
	at -10° followed by addition of H2O to give 68% Me				
	S-2-oxo-4-phenyl-3-phthalimidobutyrate. The latter was reduced with LiBH4				
	in THF at -25° to give 96% Me (2R,3S)- and (2S,3S)-2-hydroxy-4-				
	phenyl-3-phthalimic	lobutyrat	e. This was	converted to cyclohex	rylnorstatine
	hydrochloride.				
ΙT	150095-77-5P 150095	-78-6P			
	DI. SDN (Synthetic	propagat	ionis PDFD /	Preparation)	

180035-77-99 (Northetic preparation); PREP (Preparation) (preparation of, as intermediate for α-hydroxy-β-aminocarboxylic acid derivative) (150095-77-5 CAPUS 2H-180indole-2-propanoic acid, 1,3-dihydro-α-hydroxy-1,3-dioxo-β-(phenylmethyl)-, methyl ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

150095-78-6 CAPLUS 2H-Isolndole-Z-propanoic acid, 1,3-dihydro- α -hydroxy-1,3-dioxo- β -(phenylmethyl)-, methyl ester, (α S, β S)- {9CI} (CA INDEX NAME)

ANSWER 1 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN 189562-45-6P 313468-87-0P 189562-45-69 313468-97-09 RE: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation) (production of aminohydroxybutyric acid decivs.) 189562-45-6 CAPJUS Benzenebutanotic acid, P-[bis(phenylmethyl)amino]-q-hydroxy-, methyl ester, (aS.AS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

313468-87-0 CAPLUS Benzenebutanoic acid, α -hydroxy- β -[(phenylmethyl)amino]-, ethyl ester, (α S, β S)- (9CI) (CA INDEX NAME)

L6 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) Absolute stereochemistry.

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L6 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2005 ACS ON STN ACCESSION NUMBER: 1992:651744 CAPLUS DOCUMENT NUMBER: 117:251744
                                                                                                                                                                                                                               117:251744
Aminodooxybestatin and epi-aminodooxybestatin:
stereospecific synthesis and aminopeptidase
inhibition
Herranz, Rosarior Vinuesa, Soledadı Castro-Pichel,
Julias Perez, Concepcion; Garcia-Lopez, H. Teresa
Inst. Quin. Med., CSIC, Madrid, 28006, Spain
Journal of the Chemical Society, Perkin Transactions
1: Organic and Bio-Organic Chemistry (1972-1999)
(1992), (14), 1825-30
CODEN: JCPRB4: ISSN: 0300-922X
Journal
      AUTHOR (S)
      CORPORATE SOURCE:
(1992), (14), 1825-30
COODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: Sournal
LANGUAGE: Reglish
OTHER SOURCE(S): CASREACT 117:251744

AB The synthesis of (25,3R)-ADPBA-L-Leu-OH (DAPBA -
2,3-diamino-4-phenylbutanoic seid) (aminodeoxybestatin) and
(2R,3R)-DAPBA-L-Leu-OH (epi-aminodeoxybestatin), bestatin and epi-bestatin
analogs, resp., in which the hydroxy group has been replaced with an amino
group, is described by two different methods. The first one
involves the synthesis of bis-(N-2)-DAPBA (2 -
benzyloxycatbonyl), by hosologation of N-2-phenylalanine, via a modified
Strecker synthesis followed by subsequent coupling with the Me
ester of L-leucine and removal of the protecting groups. Following this
procedure, 25% racemization at the C-3 center of the DAPBA derivs. took
place during the homologation reaction. The second method
involves the stereospecific SN2 nucleophilic substitution of the 2-hydroxy
group of (2R,3R) - and (2S,3R)-3-(benzyloxycarbonyl) amino-2-hydroxy-4-
phenylbutanoyl-L-leucine He esters, and subsequent saponification, aido
reduction and pi-bestatin with an amino group results in a decrease in
their aminopeptidase (AP-B, AP-M and Leu-AP)-inhibitory potencies.

II 12472-04-3P 124782-04-5P AP-M
ABLE RCT (Resctant), SNN (Synthetic preparation), PREP (Preparation), RACT
```

124792-04-39 124792-06-59 RE. RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent) (preparation and mesylation of) 124792-04-3 CAPLUS Benzenebutanotc acid, α-hydroxy-β-[[(phenylmethoxy)carbonyl]amino]-, methyl ester, (αS, βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

124782-06-5 CAPLUS Benzenebutanoic acid, α -hydroxy- β -[[(phenylmethoxy)carbonyl]ami no]-, methyl ester, $(\alpha R, \beta R)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L6 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1957:1600 CAPLUS
DOCUMENT NUMBER: 1957:1600 CAPLUS
ONCIGINAL REFERENCE NO: 51:287d-1,288a-b
TITLE: The synthesis of mandelic acid
analogs. II. Stryylglycolic acids
AUTHOR(S): Nerdel, Friedrich Rachel, Hans
CORPORATE SOURCE: Chemische Berichte (1955), 89, 671-7
CODEN: COMBEN, 15SN: 0009-2940

DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): ASREACT 51:1600
AB cf. C.A. 49, 6217e. Adding dropwise 54 cc. concentrated HCl to 80 cc.
PRCHICHCHO and 49 g. NaCN in 250 cc. Et20 cooled with ice, stirring the
mixture 1 hc. at 0 and 1 hr. at 20°, washing the filtered
give
give

Give

AND NAMEWORK (MINERAL PROPERTION OF AUTHORS AND AND AUTHORS)

AND NAMEWORK (MINERAL PROPERTION OF AUTHORS AND AUTHORS AUTHORS AUTHORS AND AUTHORS AUTHORS AND AUTHORS AUTHORS AND AUTHO 65-70% DL-PhCH:CHCH(OH)CN (I), m. 74-5°. Adding dropwise at below 10° a mixture of 250 cc. concentrated HCl and 40 cc. concentrated H2SO4 to 65-70% DL-PhCH:CHCH(CH)CN (I), m. 74-5°. Adding dropwise at below 10° a mixture of 250 cc. concentrated HCL and 40 cc. concentrated H2S04 to 90 g.

I in 200 cc. Et20, warming the mixture 0.5 hr. at 15°, and diluting it after several hrs. with 3-4 fold ice-H2O give up to 85% DL-styrylglycolic acid (II) amide, m. 141°, which (10 g.), refluxed 1 hr. with 15 g. (CO2H)2 in 200 cc. H2O, gives 80% II, m. 137°. Concentrating slowly in vacuo a mixture of 30 g. (+)-bornylamine (III) in 200 cc. Et20 and 30 g. II in 200 cc. MeOH until 2/3 of the solvents are evaporated, filtering off the precipitate, [a]D 18°, and recrystg. it 7-8 times from Me2CNOH give 20 g. III D-8tyrylglycolate, [a]D 28° (MeOH). Recrystg. the residue of the original mother liquor several times from H2O gives 10 g. III L-styrylglycolate, [a]D 26° (MeOH).

Recrystg. the residue of the original mother liquor several times from H2O gives 10 g. III L-styrylglycolate, [a]D 26°.

Hydrogenation of D-II in MeOH 5 min. with Pt02 gives 100% (+)-m-hydroxy-phenylbutyric acid (IV), m.

114-15°, [a]D20 10.4° (Et0B). Refluxing 4.5 g. IV in 135 cc. absolute MeOH 16 hrs. with 5 cc. concentrated H2S04 gives 4 g. Me ester (V),

b16 155-7°, [a]D20 23° (CGH6). Shaking 3 g. V 6 hrs. with 50 cc. supersatd. NH3-NH4OH gives the amide (VI), needles, m. 124°, [a]D20-71° (MeOH). DL-amide, m. 130°.

Bromination of D-II in CHC13 gives (-)-α-hydroxy-β-γ-dibromo-γ-phenylbutyric acid (VII). m. 177° (decomposition), [a]D20-60° (MeOH). Condensation of 36 g. m-O2MCGN4CHCHCHCRO in 300 cc. CHC13 with 42 g. MaCN and 22 cc. 35.4% HCl as above gives 70-80% (3-nitrostyryl)glycolic acid (VIII) nitrile (IX), m. 16-8°, which treated with Bc1 and CSH5N, gives the 0-Bz derivative, m. 111°. Treating 32 g. IX in 200 cc. Et20 with 79 cc. concentrated HCl and 12.6 cc. concentrated H2S04 3 days at 20°, pouring the mixture into ice-H20, extracting with 8t20, and recrystg. the residue of the Et20 extract give 20-22 g. VIII, slightly yellow needles, m. 130-5° (decomposition), which, treated with Bc1 m CHC1 L6 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Absolute stereochemistry.

144676-51-7 CAPLUS Benzenebutancic acid, α -[(methylaulfonyl)oxy]- β -[([(phenylmethoxy)carbonyl]amino]-, methyl ester, {R-(R*,R*)}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 4 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) actd, m. 113*, [e]D20 10.6*. Hydrogenation of c. EtOH vith 2 0.9. β-phenylglycidic metal Et ester in 50 cc. EtOH vith 2 0.7. Acts 10.2 and atm. pressure gives PhcH2CH(OH)CO2Et, b16 153*, which, sapond, with NaOEt, gives the free actd, m. 95 (Ac deriv., m. 72', andde, m. 112'). The equil. consts. of the m- and p-substituted PhCOMe are detd. to be, resp.: NO2, 0.43, 0.28; Br. 0.77, 1.2*, Med., 1.27, 7.4; NHAc, 1.31, 6; Me, 1.53, 3; OH, 1.47, 14; H, 1.52, 1.52; NH2, 1.73, 18; PhCH:CHCHO, 0.032; 3-ONCARDAMO, 0.43. The rotation dispersions of D-II, VI, VII, and VIII in MeCH, EtOH, dioxane, Me2CO, AcOH, and NaOH are given in tables.

7226-82-6, Butyric acid, 2-hydroxy-4-phenyl-, methyl ester

ester (preparation of)
7226-82-6 CAPLUS
Benzenebutanoic acid, \(\alpha \text{-hydroxy-, methyl ester (9CI)} \) (CA INDEX NAME)

о он || | |- С-- СН-- СН2-- СН2-- Рh

=> s 15 and nitrile 55666 NITRILE 25916 NITRILES 70084 NITRILE

(NITRILE OR NITRILES)
7 L5 AND NITRILE

L7

=> d ibib abs hitstr tot

L7 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 2004:700272 CAPLUS DOCUMENT NUMBER: 141:174475

TITLE:

141:174475
Process for producing erythro-3-amino-2hydroxybutyric acid derivatives
Furukawa, Yoshiro: Yaegashi, Keisuke: Hinoue, Kazumasa
Daiso Co., Ltd., Japan
Eur. Pat. Appl., 12 pp.
CODEN: EPXXDW
Patent INVENTOR (S) PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: Patent English FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

RIND DATE APPLICATION NO. PATENT NO. DATE EF 1449824 A1 20040825 EF 2004-290653 20000622
R: CH, DE, FR, GB, LI
EF 1053232 A2 20001227 EF 2000-401792 20000622
EF 1053232 A3 20010307
R: AT, BE, CH, DE, DX, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO
PRIORITY APPLN: INFO:

FRIORITY APPLN: INFO:

JP 1999-174967 EP 2000-401792 CASREACT 141:174475; MARPAT 141:174475 A 19990622 A3 20000622 OTHER SOURCE(S):

A process for producing an erythro-3-amino-2-hydroxybutyric acid derivative involves reaction of a 2-amino aldehyde derivative I [R1 is

c, cycloalkyl, alkylthio, arylthio or (un)substituted aryl, Pl, P2 are (un)substituted aralkyl, alkyloxycarbonyl, arylcarbonyl or arylsulfonyl) with a metal cyanide in the presence of an acid chloride and/or an acid anhydride to give stereoselectively an erythro-3-amino-2-bydroxybutyronitrile derivative II (same R1, Pl and P2; R2 is alkylcarbonyl

(un) substituted arylcarbonyl group]. The mitrile derivative II is treated with an acid in water or aqueous solvent to convert it into an erythro-3-amino-2-hydroxybutyric acid derivative III [same R1; R3 is H; Q1,

are H, (un) substituted analkyl or arylsulfonyl) or with an acid in an alc. solvent R3OH to convert it into an ester III [same R1, Q1 and Q2; R3 is alkyl, cycloalkyl or (un) substituted analkyl; under two-phase catalysis. Thus, the process was applied to the synthesis of Me

L7 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 2002:444539 CAPLUS
DOCUMENT NUMBER: 137:33079
TITLE: Process for preparation of α-hydroxy amides and related α-hydroxy carbonyl compounds by, e.g., condensation of carbonyl compounds by, e.g., condensation of carbonyl compounds by, elg., condensation of carbonyl comp Patent

DOCUMENT TYPE: LANGUAGE: English FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE B1 20020611 US 2001-794140 US 2000-185399P CASREACT 137:33079; MARPAT 137:33079 US 6403818
PRIORITY APPLN. INFO.:
OTHER SOURCE(S): 20010228 P 20000228

$$\label{eq:h3C} \textbf{H}_{3}\textbf{C} - \hspace{-1.5cm} \begin{array}{c} \text{OH} & \text{O} & \text{H} \\ \text{I} & \text{II} & \text{I} \\ \text{CH} - \text{C} - \text{N} - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_3 \\ \end{array} \\ \text{IV}$$

A novel process is disclosed for the one-pot preparation of a-hydroxy carbonyl compds. (mostly a-hydroxy anides) of formula I and their derivs. via the condensation of II and III in the presence of R3-TH (herein: Y = O, S, NRG (R6 = H, OH, alkyl, alkoxy, cycloalkyl, alkenyl, alkynyl, or (un)substituted 5- to 12-membered heteroaryl group, etc.); R1, R2 independently = H, alkyl, alkoxy, cycloalkyl, bitcycloalkyl, alkenyl, alkynyl, heteroaryl or (un)substituted 5- to 12-membered heteroaryl group, etc.; R3 = H, OH, alkyl, alkoxy, cycloalkyl, alkenyl, alkynyl, aryl, (un)substituted 5 to 12-membered heteroaryl group, etc.; R4 = H, Substituted 5 to 12-membered heteroaryl group, etc.; R4 = H, substituted silvy protecting group (preferably -51Me3, -51Me2tBu or 51FA2tBu), alkanoyl, alkenoyl, alkenoyl, alkynoyl, aryl, heteroaryloyl, etc.; R5 = substituted silvy protecting group (preferably -TMS, -TBDMS or -TBDPS), alkanoyl, alkenoyl, alkynoyl, aryloyl, heteroaryloyl, etc.). A key intermediate in the proposed process is the corresponding acyl cyanide, generated in situ from condensation of II and III. For example, to a stirred solution of 4-methylbenzaldehyde (1.0 mmol) and dinitrile III (R4 = tet-butyldimethylsiyl, 1.2 mmol) in one portion. After 5 min, a solution of tetrabutylammonium fluoride in THF (1.5 mmol) was added dropwise and the reaction stirred at 0° for an addni. 20 min. The solution was concentrated and purified via silica gel column chromatog. to provide hydroxyacetamide IV as colorless powder in 94% yield. Approx. 75 specific examples of I were prepared The invention is proposed to be useful for the production of

ANSVER 1 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) (25,35)-3-(dibenzylamino)-2-hydroxy-4-phenylbutyrate (erythro:threo = 97:13, 73% yield) starting from N,N-dibenzyl-L-phenylalaninal. 189562-45-69 313468-67-09

lubse2-45-69 313468-97-09
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(production of aminohydroxybutyric acid derivs.)
199562-45-6 CAPJUS
Benzenebutanoic acid, P-[his(phenylmethyl)amino]-a-hydroxy-,
methyl ester, (aS, \$S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

313468-87-0 CAPLUS Benzenebutanoic acid, α -hydroxy- β -[(phenylmethyl)amino]-, ethyl ester, (aS, β S)- (9CI) (CA INDEX NAME)

ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) statine analogs. The invention process gives products similar to the Passerini reaction, but uses amines instead of isocyanides, and

to the Passerini reaction, but uses amains a second and also gives higher yields.
342389-98-49 342390-00-59 433344-70-0P, Methyl
2-[(tect-butyldimethylsilyl)oxy]-4-phenylbutanoate
RL: IMF (Industrial manufacture), SPN (Synthetic preparation), PREP (Preparation)

(Pteparation)
(products preparation of α-hydroxy carbonyl derivs. and related
compds. by condensation of carbonyl compds.,
(silyloxy)propanedinitriles, and amines)
342389-98-4 CAPLUS
Benzenebutanoic acid, α-[((1,1-dimethylethyl)dimethylsilyl)oxy]β-[[(penylmethoxy)carbonyl]amino]-, methyl ester,
(αR,βS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

342390-00-5 CAPLUS Benzenebutanoic acid, $\alpha-[\{(1,1-\text{dimethylethyl})\text{dimethylsilyl}]\text{oxy}]-p-[\{(phenylmethoxy)\text{carbonyl}]\text{amino}]-, methyl ester, (aR,<math>\beta$ R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

435344-70-0 CAPLUS Benzenebutanoic acid, $\alpha-\{[(1,1-dimethylethyl)dimethyleilyl]oxy\}-, methyl ester (9CI) (CA INDEX NAME)$

L7 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

REFERENCE COUNT

THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:
1993:550824 CAPLUS
119:160824
119:160824
119:160826
1ITILE: PROMOTION OF THE PROMOTION OF T PATENT INFORMATION: PATENT NO. KIND DATE APPLICATION NO. DATE A2 A3 EP 543343 A2 19930526 EP 1992-119634 19921117

R: AT, BE, CH, DE, FR, GB, LT, LI, NL, SE
JP 06184069 A2 19940705 JP 1992-303629 19921113

CA 2083108 AA 19930520 CA 1992-2083108 19921117

RITY APPLIN. INFO:
CH 1991-3373 A 19911119

RE SOURCE(S):
CASREACT 119:160824; MARPAT 119:160824

RLCH(NR3R)CH(OH)CO2R2 (R1 = (substituted) alkyir R2 = H, alkyir R3, R4 = H, protecting group R3M = bifunctional protecting group, were prepared by 1 treatment of RLCH(NR5R6)COX (R5,R6 = R3,R4, except that both R5,R6 cannot = H; X = Br, Cl) with Me33iCN to give RLCH(NR5R6)COX (2) conversion of the nitrile to RICH(NR5R6)COXCO2R7 (R7 = alkyi), 3) selective reduction of the keto group, and 4) optional deprotection/ester hydrolysis. Thus, N-phthaloyl-L-phenylalanine was refluxed with SCC12 to give 98% acid chloride, which was heated with Me35ICN and Zn12 in 7HF to give 87% nitrile. This in EE2C/MeOH/HCL was stirred at -10° followed by addition of H2O to give 68% Ne S-2-oxo-4-phenyl-3-phthaliandbutyrate. The latter was reduced with LHBH in THF at -25° to give 96% Ne (2R, 3S) - and (2S, 3S)-2-hydroxy-4-phenyl-3-phthaliandbutyrate. This was converted to cyclohexylnorstatine hydrochloride. EP 543343 EP 543343 19930526 EP 1992-119634 19921117 PRIORITY APPLN. INFO.: OTHER SOURCE(S): hydrochloride. 150095-77-5P 150095-78-6P 150095-77-59 150095-78-69 RE: SPN (Synthetic preparation); PREF (Preparation)
(preparation of, as intermediate for α-hydroxy-β-aminocarboxylic acid derivative)
150095-77-5 CAPLUS
2H-1soindole-2-propanoic acid, 1,3-dihydro-α-hydroxy-1,3-dioxo-β-(phenylmethyl)-, methyl ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

150095-78-6 CAPLUS 2H-1soindole-2-propanoic acid, 1,3-dihydro- α -hydroxy-1,3-dioxo- β -(phenylmethyl)-, methyl ester, (α S, β S)- (9CI) (CA INDEX NAME)

L7 ANSVER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:228191 CAPLUS
DOCUMENT NUMBER: 12281272
TITLE: Sitrile oxide [3 + 2] cycloaddition:
application to the synthesis of
6-substituted 3(2H)-pyridazinones and 6-substituted
4,5-dihydro-4-hydroxy-3(2H)-pyridazinones
Baraldi, P. G.: Bigoni, A.: Cacciari, B.: Caldari, C.:
Manfredini, S.: Spalluto, G.
CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Univ. di
Ferrara, Ferrara, 1-44100, Italy
SOURCE: Synthesis (1994), (11), 1158-62
CODEN: SYNTBF: ISSN: 0039-7881

PUBLISHER: Thiese
DOCIMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:81272
AB An efficient method for the preparation of 6-substituted
3(2H)-pyridazinones starting from 3,5-disubstituted 4,5-dihydroisoxazoles is
described. N-O bond cleavage of the isoxazoline ring promoted by
molybdenum hexacarbonyl or by catalytic hydrogenation afforded the
a-hydroxy y-keto esters RCOCHECH(OR)COZET (I, R = Me. Bu, Z-,
4-pyridyl, 4-ROCGH4) which were converted into 6-substituted
4,5-dihydro-4-hydroxy-3(2H)-pyridazinones on treatment with hydrazine hydrate at room temperature
or
reflux in high yield starting from I. An intramol. version of this reflux in high yield starting from I. An intramol. version of this methodol. has been developed to prepare the known antiulcer tricyclic 5H-[1]-benzopyrano[4,3-c]pyridazin-3(2H)-one. 160427-19-OP RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (aittria exide [3 + 2] cycloaddn. to pyridazinones) 160427-19-0 CAPLUS Benzenebutanoic acid, u,4-dihydroxy-y-oxo-, ethyl ester (9CI) (CA INDEX NAME)

(Continued) L7 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

L7 ANSVER 5 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 1992:651744 CAPLUS DOCUMENT NUMBER: 117:251744
TITLE: Animales

Aminodeoxybestatin and epi-aminodeoxybestatin: stereospecific synthesis and aminopeptidase

inhibition

inhibition
Herranz, Rosarior Vinuesa, Soledad; Castro-Pichel,
Julia; Perez, Concepcion; Garcia-Lopez, M. Teresa
Inst. Quis. Med., CSIC, Madrid, 28006, Spain
Journal of the Chemical Society, Perkin Transactions
1: Organic and Bio-Organic Chemistry (1972-1999)
(1992), (14), 1825-30
CODEN: JCPRB4: ISSN: 0300-922X AUTHOR(S): CORPORATE SOURCE:

DOCUMENT TYPE: LANGUAGE:

OTHER SOURCE(S):

(1992), [18], [182-30

CODEN: JCRRHA 155N: 0300-922X

MEMOTITYPE: Journal

UAGE: English

R SOURCE(S): CASREACT 117:251744

Land Carrier Control Control Control Control

2,3-diamino-4-phenylbutanoic acid) (aminodeoxybestatin) and

(2R, RR-DAPA-1-Leu-OH (epi-aminodeoxybestatin), bestatin and epi-bestatin

analogs, resp., in which the hydroxy group has been replaced with an amino

group, is described by two different methods. The first one

involves the synthesis of bis-(N-2)-DAPAA (2 =

benzyloxycarbonyl), by homologation of N-2-phenylalanine, via a modified

Streeker synthesis of cilowed by subsequent coupling with the Me

ester of L-leucine and removal of the protecting groups. Following this

procedure, 25t racemization at the C-3 center of the DAPAA derivs, took

place during the homologation reaction. The second method

involves the stereospecific SN2 nucleophilic substitution of the 2-hydroxy

group of (2R, SR) - and (2S, SR) -3-(benzyloxycarbonyl) amino-2-hydroxy-4
phenylbutanoyl-L-leucine Me esters, and subsequent saponification, around for the Narroscotic SN2 Narroscotics of the budgers around for the Narroscotics of the budgers around for the Narroscotics of the protection of the Narroscotics of the budgers around for the Narroscotics of the protection of the Narroscotics of the budgers around for the Narroscotics of the protection of the Narroscotics of the protection of the Narroscotics of the protection of the protection of the Narroscotics of the

pnemyLourancy1-L-Isutine Re esters, and subsequent saponification, sized reduction and removal of the N-2-protecting group. Replacement of the hydroxy group of bestatin and epi-bestatin with an amino group results in a decrease in their aminopeptidase (AP-B, AP-H and Leu-AP)-inhibitory potencies.

IT 124782-04-39 124782-06-59

124782-04-39 124782-06-5P (Synthetic preparation); PREP (Preparation); RACT (Reactant) of SPN (Synthetic preparation); RACT (Reactant) or reagent) (preparation and mesylation of) 124782-04-3 CAPLUS Benzemebutanoic acid, α-hydroxy-β-[[(phenylmethoxy)carbonyl]ami no]-, methyl ester, (α5,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

124782-06-5 CAPLUS Benzenebutanoic acid, «-hydroxy-β-[[[(phenylmethoxy)carbonyl]amino]-, methyl ester, («R, RR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L7 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 1989:594247 CAPLUS COCUMENT NUMBER: 111:194247

Lipase-catalyzed irreversible transesterification

AUTHOR(S):

Lipase-catalyzed irreversible transesterification using enol esters: resolution of cyanohydrins and syntheses of ethyl (R)-2-hydroxy-4-phenylbutyrate and (S)-propranolol wang, Yi Fongi Chen, Shui Tein; Liu, Kevin K. C.; Wong, Chi Huey
Dep. Chem., Texas A and M Univ., College Station, TX, 7843, USA
Tetrahedron Letters (1989), 30(15), 1917-20
CODEN: TELEAY; ISSN: 0040-4039
Journal
English
CASREACT 111:194247 CORPORATE SOURCE:

DOCUMENT TYPE:

LANGUAGE: OTHER SOURCE(S): GI

Racemic hydroxyacetonitriles, (±)-I, (±)-PhCH2CH2CH(OH)CN, and (±)-PhCH2CC3CH(OH)CN, were resolved by lipoprotein lipase. (±)-I gave (+)-I which was sequentially reduced (LiAlH4) and treated with Me2CO and NaBH4 to give (S)-propranolol. 90318-82-5p

90318-82-39
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
90318-82-5 CAPLUS
Benzenebutanoic acid, a-hydroxy-, ethyl ester, (aR)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

ANSWER 5 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

144676-50-6P 144676-51-7P

144676-50-69 144676-51-79
RE: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(preparation and substitution reaction of, with azide)
144676-50-6 CAPLUS
Benzenebutanoic acid, a-[(methylsulfonyl)oxy]-β[(phenylmethoxy)carbonyl]amino]-, methyl ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

144676-51-7 CAPLUS

Benzenebutanoic acid, a-{(methylsulfonyl)oxy]-β-[((phenylmethoxy)carbonyl)amino]-, methyl ester, [R-{R*,R*}]- (9CI) (CA RNDEX NAME)

Absolute stereochemistry.

L7 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1957:1600 CAPLUS
DOCUMENT NUMBER: 1957:1600 CAPLUS
ONIGINAL REFREIENCE NO.: 51:287d-1,288a-b
TITLE: The synthesis of mandelic acid analogs. II.
Strytglycolic acids
AUTHOR(S): Nerdel, Friedrich Rachel, Hans
CORPORATE SOURCE: Chemische Berichte (1956), 89, 671-7
CODEN: CHEMENT 15SN: 0009-2940

JOURNAL LANGUAGE: Journal LANGUAGE: Journal LANGUAGE: Unavailable
OTHEM SOURCE(S): ASKERACT 51:1600
Ab cf. C.A. 49, 6217e. Adding dropwise 54 cc. concentrated HCl to 80 cc.
PhCHICHCHO and 49 g. NaCN in 250 cc. Et20 cooled with ice, stirring the mixture 1 hc. at 0 and 1 hr. at 20', vashing the filtered
give 67.00 by NaCN (10 c) and 10 capture to 10 and 1 hr. at 20', vashing the filtered

65-70% DL-PhCH:CHCH(OH)CN (I), m. 74-5°. Adding dropwise at below 10° a mixture of 250 cc. concentrated HCl and 40 cc. concentrated H2504 to

10° a mixture of 250 cc. concentrated HC1 and 40 cc. concentrated H2504 to 10° a mixture of 250 cc. concentrated HC1 and 40 cc. concentrated H2504 to after several hrs. with 3-4 fold ice-H20 give up to 858 DL-styrylglycolic acid (II) amide, m. 141°, which (10 g.), refluxed 1 hr. with 15 g. (CO2H)2 in 200 cc. H20, gives 80% II, m. 137°. Concentrating slowly in vacuo a mixture of 30 g. (+)-bornylamine (III) in 200 cc. Et20 and 30 g. II ozo Co. Et20 and 30 g. II in 200 cc. H80H until 2/3 of the solvents are evaporated, filtering off the precipitate, (a)D 18°, and recrystg. tt-9 times from H20CHG give 20 g. III D-styrylglycolate, (a)D 28° (MeOH). Recrystg. the residue of the original mother liquor several times from H20CHG give D-II, m. 139° (decomposition), (a)D 100° (MeOH), and L-II (-)-isomer, m. 139°, (a)D -98°. Hydrogenation of the salts gives D-II, m. 139° (decomposition), (a)D 100° (MeOH), and L-II (FOCH). Refluxing 4.5 g. IV in 135 cc. absolute MeOH 16 hrs. with 5 cc. concentrated H2504 gives 4 g. Ne ester (V), b)6 155-7°, [a)D20 22° (CGH6). Shaking 3 g. V 6 hrs. with 50 cc. supersatd. NH3-NH40H gives the amide (VI), needles, m. 124°, [a)D20 -37° (MeOH). DL-amide, m. 130°. Bromination of D-II in CHC13 gives (-)-a-hydroxy-p, y-dibromo-y-phenylbutyric acid (VII), m. 171° (decomposition), [a)D20 -60° (MeOH). Condensation of 36 g. m-O2NCCH4CH:GCH30 in 300 cc. CHC13 with 42 g. NaCN and 22 cc. 35.4 HCl as above gives 70-80% (3-nitrostyrylglycolic acid (VIII) mitrie (IX), m. 76-8°, which, treated with B2cl and CSHSN, gives the 0-B2 derivative, m. 111°. Treating 32 g. IX in 200 cc. Et20 with 79 cc. concentrated H2504, extracting with Et20, and recrystg.

200 cc. Et2O with 79 cc. concentrated HCl and Ir.o cc. concentrated news sat 20°, pouring the mixture into ice-H2O, extracting with Et2O, and recrystg. the residue of the Et2O extract give 20-22 g. VIII, slightly yellow needles, m. 130-5° (decomposition), which, treated with Br in CHCl3, gives α-hydroxy-β,γ-dibromo-γ-(3-nitrophenyl)butyric acid, m. 175-6° (decomposition). Resolution of VIII with III gives a III (+)-VIII salt, [α]D2O 24° (MeOH), from which the free (+)-VIII, m. 112-17', [α]D2O 17', is obtained on decomposition with HCl. Hydrogenation of (+)-VIII in MeOH with PtO2 gives (+)-α-hydroxy-γ-(3-minophenyl)butyric acid (not quite pure), [α]D2O 0.75° (MeOH), which, diazotized and treated with CUZHZ, gives (+)-α-hydroxy-γ-phenylbutyric acid, m. 113°, [α]D2O 10.6°. Hydrogenation of 20 g. β-phenylglycidic acid Et ester in 50 cc. EtOH with 2 g. Raney Ni 8

L7 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) hrs. at 20° and atm. pressure gives PhCH2CH(OH)COZEt, b16 153°, which, sapond. with NaOEt gives the free acid, m. 96° (Ac deriv., m. 72°, anide, m. 112°). The equil consts. of the m- and p-substituted PhCOMe are detd. to be, resp: NO2, 0.43, 0.28; Br, 0.77, 1.2; NeO, 1.27, 7.4; NHAC, 1.31, 6; Ne, 1.53, 3; OH, 1.47, 14; H, 1.52, 1.52; NH2, 1.73, 18; PhCH:CHCHO, 0.032; 3-NO2 analog, 0.023; 3-OXGENCOMe, 0.43. The rotation dispersions of D-II, VI, VII, and VIII in MeOH, EtOH, dioxane, MeZCO, AcOH, and NaOH are given in tables.

17 7226-82-5, Butyric acid, 2-hydroxy-4-phenyl-, methyl ester (preparation of)

RN 7226-82-6 CAPLUS

CR Benzenebutanoic acid, a-hydroxy-, methyl ester (9CI) (CA INDEX NAME)